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Technical Report - Methods: A diagnostic approach to analyze the direction of change in model outputs based on global variations in the model inputs

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Key Points:

- We bring attention to a diagnostic strategy – assessing the direction of change, which quantifies whether the increase (or decrease) of a model input leads to a positive (or negative) change in a model output variable.
- We developed a quantification and visualization approach to analyze the direction of change due to input variability within a Global Sensitivity Analysis context.
- We demonstrated our approach as a time-varying analysis to diagnose how the parameters of a widely used hydrological model control the output's direction of change.

Abstract

Hydrologic models are used to simulate natural phenomena while making different assumptions about the levels of complexity with which natural processes should be represented. Global Sensitivity Analysis is regularly applied to understand how the inputs (including forcing, parameters and initial states) of these models control their outputs. A less widely explored strategy to support such diagnostic analysis is the assessment of direction of change (DOC) which addresses the question whether the increase (or decrease) of a model input leads to a positive (or negative) change in the model output. We propose a metric, called Direction Index, to quantitatively assess the direction of change and develop an approach to calculate it. The basic idea of our approach is two-folded: (1) Estimate the zero-th and first order term of the High Dimensional Model Representation (HDMR) decomposition. (2) Calculate the derivatives of the first order term of the HDMR decomposition with respect to a given input. We demonstrate our approach on a widely used conceptual lumped hydrological model (Hymod) with a time-varying analysis applied to the Leaf River Catchment in the USA. The results show that our approach provides new insights into the behaviour of the model, which can be used to guide model structure improvement or to improve calibration efficiency.

1 Introduction

Hydrological models simplify and abstract the complexity of the natural world in ways that might be more or less consistent with our assumptions about how nature works. The complexity and type of such models varies widely [Ye et al, 1997], based on different assumptions the modeler makes about how the real-world phenomena can be conceptualised and simplified. Over the years, researchers have developed different diagnostic analysis strategies to assess how hydrological models work and to identify discrepancies with the underlying system [Biondi & De Luca, 2013; Gupta et al., 2008; He et al., 2015; Hrachowitz et al., 2014; Kim et al., 2015; Li et al., 2013; Milella et al., 2012; Trudel et al., 2014; Wagener et al., 2003; Wagener & Gupta, 2005; Wright et al., 2018]. Diagnostic strategies include methods to assess model performance and behaviour in a hydrologically interpretable way. Strategies to do so include the use of hydrologic signatures; and time-varying or time-averaged Global Sensitivity Analysis (GSA) methods to understand what model inputs (including forcing, parameters and initial states), and thus what modelled processes, control the model output [Gupta et al., 2008; Cheng et al., 2019; Cloke et al., 2008; Euser et al., 2013; Ghasemizade et al., 2017; Haghnegahdar et al., 2017; Hu et al., 2015; Vanrolleghem et al., 2015; Van Werkhoven et al., 2008; Wagener & Kollat, 2007; Zhan et al., 2013].

A little explored strategy to support such diagnostic analysis is the assessment of direction of change (DOC) originally proposed by Samuelson [1941]. Samuelson's work was aimed at determining “*the equilibrium values of given variables (unknowns) under postulated conditions (functional relationships) with various data (parameters) being specified*”. To achieve this, he claimed that “*In order for the analysis to be useful it must provide information concerning the way in which our equilibrium quantities will change as a result of changes in the parameters taken as independent data.*” His approach thus addresses the question whether the increase (or decrease) of a model input leads to a positive (or negative) change in the model output variable.

In Samuelson's work, the direction of change is measured through the signs of the partial derivatives of the output with respect to each input. Following similar ideas, others have

investigated the direction of change by computing and plotting the derivatives using a One-At-a-Time (OAT) design (see review in *Borgonovo and Plischke's* [2016]). For example, *Borgonovo* [2010] developed an OAT method based on the functional analysis of variance (ANOVA) decomposition of a finite change of the output and used it to assess the DOC of a probabilistic safety assessment model. *Sweetapple et al.* [2014] applied a simple OAT sensitivity analysis to a wastewater treatment plant model (the BSM2-e model) as a preliminary investigation of how the model outputs change in response to variations of different inputs. *Borgonovo et al.* [2017] calculated the output derivatives of rainfall-runoff models (using the FUSE framework) with the Distributed Evaluation of Local Sensitivity Analysis (DELSA) method [*Rakovec et al.*, 2014], and visualized them using derivative scatterplots (D-scatterplot). The existence of both positive and negative signs implied the nonmonotonicity of the DOC. *Gupta and Razavi* [2017] computed the partial derivatives of the output (streamflow) of the rainfall-runoff HBV-SASK model for each time step with an OAT design. They assessed the positive and negative derivative separately and found that different parameters may have different signs of partial derivatives while these signs also changed with time.

Different from the OAT design used in the above-mentioned studies, DOC analysis can also be performed within a GSA context, thus assessing the direction of change induced by one input while all other inputs vary simultaneously. Few studies have been carried out using such an approach. For example, *Anderson et al.* [2014] plotted the first order terms of the high-dimensional model representation (HDMR) decomposition of an integrated assessment model (the DICE model). HDMRs describe a family of multivariate representations for the input-output mapping of any model [*Rabitz*, 1999]. The first order term of the HDMR decomposition represents the independent effect of a given input on the model output. *Borgonovo et al.* [2017], besides using an OAT design as mentioned above, also investigated DOC within a GSA context using two different methods. The first one plots the first order terms in the HDMR decomposition (denoted as COSI curves), which is the same approach used by *Anderson et al.* [2014]. The second one uses Cumulative Sum of Normalized Reordered Output (CUSUNORO, *Plischke*, 2010) plots. CUSUNORO plots display the average mean of the standardized output when the associated input is less than a given quantile u , with u varying between 0 and 1. In these studies, the relationships between the inputs and the outputs are found to be monotonically increasing or decreasing - most of them linearly. However, in complex hydrological models, the relationship between inputs and outputs are often non-monotonic and nonlinear. A limitation of these visualisation methods is that they can only be applied to a small number of outputs to fully capture the non-monotonicity and nonlinearity of the relationship. If one needs to assess a large number of model outputs, for example a time series, it is unrealistic to study one plot for each time step. Therefore, a more convenient approach and a better visualization strategy are needed.

The interest in analyzing the sensitivity of output time series stems from a growing body of literature that used Time-varying Sensitivity Analysis (TVSA) to analyse the temporal behaviour of hydrological models [*Cloke et al.*, 2008; *Ghasemizade et al.*, 2017; *Gupta & Razavi*, 2018; *Guse et al.*, 2014; *Hass et al.*, 2015; *Herman et al.*, 2013; *Kelleher et al.*, 2013; *Massmann et al.*, 2014; *Pfannerstill et al.*, 2015; *Pianosi & Wagener*, 2016; *Reusser et al.*, 2011; *Wagener et al.*, 2003; *Wlostowski et al.*, 2013]. In TVSA, a moving window or running mean approach is used (though often with the size of a single time step) to compute the output variable within the moving window for each time step, along with computing a set of Sensitivity Indices (SIs) for each input (mostly parameters). The advantage of using a moving window with appropriate size is that it can capture the effect of a parameter over its influential period while

balancing the negative influence of noisy data and information loss due to aggregation [Massmann *et al.*, 2014]. Most TVSA studies used ‘traditional’ SA methods (such as Sobol or FAST), which provide an aggregated SI across the input (mostly parameter) space. In some cases, the parameter is only influential when varied within a certain range, or parameters with equal SI have diverse (increasing or decreasing) effects on the model output. Or it might be that the same parameter has different effects on the model output during different time periods. To address this issue, DYNIA estimates how parameter regions controlling the model vary with time [Wagener *et al.*, 2003]. However, the approach does not provide information about the trend of the model output with respect to varying each parameter. The investigation of DOC enables a more elaborate analysis and better understanding of the model (parameter) behavior. To our knowledge, there is no study combining time-varying SA and assessment of direction of change so far, although Gupta and Razavi [2018] discussed the implications of positive and negative derivatives and highlighted the need for a methodology to quantify this impact.

In our study we develop an approach to investigate the DOC of model outputs within a GSA context, convenient to implement in a time-varying analysis. Our approach builds on the method of HDMR decomposition, but with simpler calculations and improved visualization for time series. The key output of the method is a time series of a new DOC indicator, called Direction Index (DI), for each model input. We apply our method to a widely used lumped conceptual hydrologic model and an extensively investigated dataset to demonstrate its value. The information provided by our strategy could help to: [1] diagnose whether some model parameters have changing roles during different response modes of the system and hence are inconsistent with underlying assumptions, [2] provide information to reformulate the model structure and improve its performance or at least its consistency with the real-world nature, and [3] guide the model calibration process.

2 Methodology

2.1 HDMR-decomposition

High-dimensional model representation (HDMR), introduced by Rabitz *et al.* [1999], is a set of tools to analyse the relationship between a large number of input variables (x_1, x_2, \dots, x_n) and the output (y) of a model. The HDMR decomposition assumes that the input variables are independent of each other [Beccacece & Borgonovo, 2011]. The input-output mapping of a model represented by a real-valued function $y = f(x)$ can be written in the following form [Rabitz *et al.*, 1999; Sobol', 1990]:

$$f(x) = f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{1 \leq i < j \leq n} f_{ij}(x_i, x_j) + \dots + f_{12\dots n}(x_1, x_2, \dots, x_n) \quad (1)$$

where f_0 is a constant representing the mean effect (zeroth order), $f_i(x_i)$ is the first order effect of variable x_i representing the independent effect of x_i on the model output, $f_{ij}(x_i, x_j)$ is the second order effect representing the interactive effects of x_i and x_j on the model output and so on.

HDMR is commonly constructed either using cut-HDMR, which depends on the value of $f(x)$ at a reference point \bar{x} , or RS (random sample)-HDMR, which depends on the average value of $f(x)$ over the whole input variability space. In this study, RS-HDMR was used because it is

computationally more efficient for models that have more than 10 inputs and the sample size required for its approximation is not directly dependent on the input space dimension [Ziehn & Tomlin, 2009]. Firstly, the input variables are rescaled in the range [0, 1]. The input domain of function f then becomes the unit hypercube $K^n = \{(x_1, x_2, \dots, x_n) | 0 \leq x_i \leq 1, i = 1, 2, \dots, n\}$ and the terms of Eq. (1) can be reconstructed through the following expressions:

$$f_0 = E_X[f(X)] = \int_{K^n} f(X) dX \quad (2)$$

$$f_i(x_i) = E_X[f(X) | X_i = x_i] - f_0 = \int_{K^{n-1}} f(X) dX^i - f_0 \quad (3)$$

$$\begin{aligned} f_{ij}(x_i, x_j) &= E_X[f(X) | X_i = x_i, X_j = x_j] - f_i(x_i) - f_j(x_j) - f_0 = \\ &= \int_{K^{n-2}} f(X) dX^{ij} - f_i(x_i) - f_j(x_j) - f_0 \end{aligned} \quad (4)$$

...

Where dX^i is the product $dx_1 dx_2 \dots dx_{i-1} dx_{i+1} \dots dx_n$, dX^{ij} is the product $dx_1 dx_2 \dots dx_{i-1} dx_{i+1} \dots dx_{j-1} dx_{j+1} \dots dx_n$.

2.2 Definition of the Direction Index

The direction of change in the output with respect to a given input variable, x_i , is obtained through the investigation of the terms $f_0 + f_i(x_i)$ [Anderson et al., 2014]. Notice that, by rearranging the terms of Equation 3, we get:

$$E_X[f(X) | X_i = x_i] = f_i(x_i) + f_0 \quad (5)$$

Therefore, $f_i(x_i) + f_0$ represents the conditional expectation of $f(x)$ as a function of x_i , i.e. it captures the direct dependence of the output on one specific input variable while averaging all possible values of the remaining variables. In order to quantitatively represent the direction of change, we introduce a Direction Index (DI), which is calculated as the angle of the tangent at each point of the curve $f_i(x_i) + f_0$:

$$DI_i(x_i) = \arctan f_i'(x_i) \quad (6)$$

where $f_i'(x_i)$ is the derivative of $f_i(x_i)$ (i.e. of $f_i(x_i) + f_0$) at x_i . By definition, DI_i varies between -90° and 90° and measures how much the output increases or decreases when the i -th input is changed along its range of variability. The sign of DI_i represents the direction of change while the absolute value of DI_i represents the magnitude of this change. An illustrative example is given in Figure 1.

2.3 Approximation of the HDMR components

The analytical computation of each HDMR component is too difficult for complex models such as typical hydrological models. The RS-HDMR approach provides an approximation of the HDMR component in a convenient and efficient way. It is initiated by generating N sets of input samples X^S , and then evaluating the model using these samples to get model outputs $f(X^S)$. The zeroth order term f_0 is approximated by the average value of all the output samples:

$$f_0 = \int_{K^n} f(X) dX \approx \frac{1}{N} \sum_{s=1}^N f(X^s) \quad (7)$$

The first order term $f_i(x_i)$ is approximated by a linear combination of analytical basis functions. Orthonormal polynomials are selected as basis functions in this study because their use has been shown to reduce sampling costs considerably [Li *et al.*, 2002]. The linear combination is expressed in the following form:

$$f_i(x_i) \approx \sum_{r=1}^k \alpha_r^i \varphi_r(x_i) \quad (8)$$

where k is the order of the polynomial expansion, α_r^i are constant coefficients to be determined, and $\varphi_r(x_i)$ are the orthonormal basis functions. The orthonormal polynomials $\varphi_r(x_i)$ have a zero mean and unit norm and are mutually orthogonal.

The expansion coefficients α_r^i can be determined via Monte Carlo integration [Li *et al.*, 2002], in the form of:

$$\alpha_r^i = \frac{1}{N} \sum_{s=1}^N f(X^s) \varphi_r(X_i^s) \quad (9)$$

The accuracy of the approximation is determined by the error of the MC integration. Using a small sample may lead to higher inaccuracy. Variance reduction methods can be applied to improve the accuracy of the Monte Carlo integration, and hence the estimation of the expansion coefficients, without adding extra samples. The correlation method [Li *et al.*, 2003] and the ratio control variate method [Li & Rabitz, 2006] are commonly used approaches. Both methods involve an iterative process and an analytical reference function $h(x)$ to approximate $f(x)$. For example, $h(x)$ could be the truncated RS-HDMR expansion whose expansion coefficients are calculated using direct MC integration. In this study, we use the ratio control variate method because it was reported to be more stable than the correlation method [Li & Rabitz, 2006].

Normally, the polynomial order (k) for each first-order term of the HDMR decomposition (i.e. for each input) should be chosen separately. Here we use an optimisation method developed by Ziehn and Tomlin [2008] which automatically selects the optimal polynomial order for each first-order term. The idea of the method is to calculate the sum of the squared differences between the output samples and the polynomials of Eq. (7) with different orders. The smallest sum of squared errors indicates the best approximation, and the corresponding order k is chosen (For more details refer to Ziehn and Tomlin [2008]). However, in our application we have observed an over-fitting issue in the implementation of this method. Sometimes, the first-order term of the HDMR decomposition seemed to be unnecessarily “sophisticated”. To resolve the problem, at the time step where an over-fitting issue occurs, we stop using the variance reduction method and determine the expansion coefficients solely using Eq. 9. Detailed descriptions of the over-fitting issue and our solution are given in the Supporting Information.

2.4 Rescaling the output variables

Because the first step in the HDMR approach is to rescale the input variables in the domain $[0, 1]$, a scaling issue may be encountered when computing the slope of $f_i(x_i)$, as the model output (y) may vary over a much larger range. For example, in our application the output is river discharge, and the order of magnitude of first-order terms in high flow periods can reach 3 (mm/day), which leads to a slope angle close to 90 degree. This issue is also stated in *Gupta and Razavi's* [2018] work. To resolve this issue, the output of the model is also rescaled in the domain $[0, 1]$ before applying our method, so that input and output have the same order of magnitude.

2.5 General procedures for approximating Direction Indices

The general procedures to investigate the direction of change of model output with respect to input change is stated as follows:

- (1) Generate N input samples, and execute the model using sampled sets of inputs.
- (2) Rescale both inputs and output in the range $[0, 1]$, using the following equation:

$$X_s = \frac{\max(X_s) - X_s}{\max(X_s) - \min(X_s)} \quad (10)$$

- (3) For each input, estimate the zeroth and first order term of the HDMR decomposition ($f_i(x_i) + f_0$) using the method stated in 2.3.
- (4) For each input, approximate the derivatives of $f_i(x_i)$ using the derivatives of Eq. (8), and therefore approximate Eq. (6) by:

$$DI_i = \arctan \sum_{r=1}^k \alpha_r^i \frac{d\varphi_r(x_i)}{dx_i} \quad (11)$$

In a Time-varying Sensitivity Analysis context, sampling and model execution only need to be done once for all sampled input sets, and then the procedures (2)-(4) are repeated for each time step and window size.

2.6 Visualization of the results

Anderson et al. [2014] plot the first order term of the HDMR decomposition to qualitatively show the direction of change of the output variables. This is effective for a single output. However, when a time series is studied, it would be inconvenient to produce and investigate one plot for each time step. Our methodology calculates the derivative of the first order term and transform it into the angle of the tangent, which enables a quantitative assessment of the direction of change. Then, the angle of the tangent can be plotted in a colormap where the horizontal axis represents time and the vertical axis represents the input value (Fig. 1).

The example in Figure 1 uses a well-known analytical function, the Ishigami-Homma function [*Ishigami & Homma*, 1990], modified as a time-changing function as expressed below:

$$f(x, t) = \sin\left(x_1 + t * \frac{\pi}{4}\right) + a \sin^2\left(x_2 + t * \frac{\pi}{8}\right) + bx_3^4 \sin\left(x_1 + t * \frac{\pi}{8}\right) \quad (12)$$

where the three inputs x_i ($i=1,2,3$) are drawn from a uniform distribution in the range $(-\pi, \pi)$ and the constant parameter are set to $a = 7$, $b = 0.1$. In this example, we generate 10,000 input samples using Latin Hypercube Sampling. The maximum polynomial order (k_{\max}) is set to 10. The ratio control variate method is applied for variance reduction. A time series of four time steps is used for a demonstration.

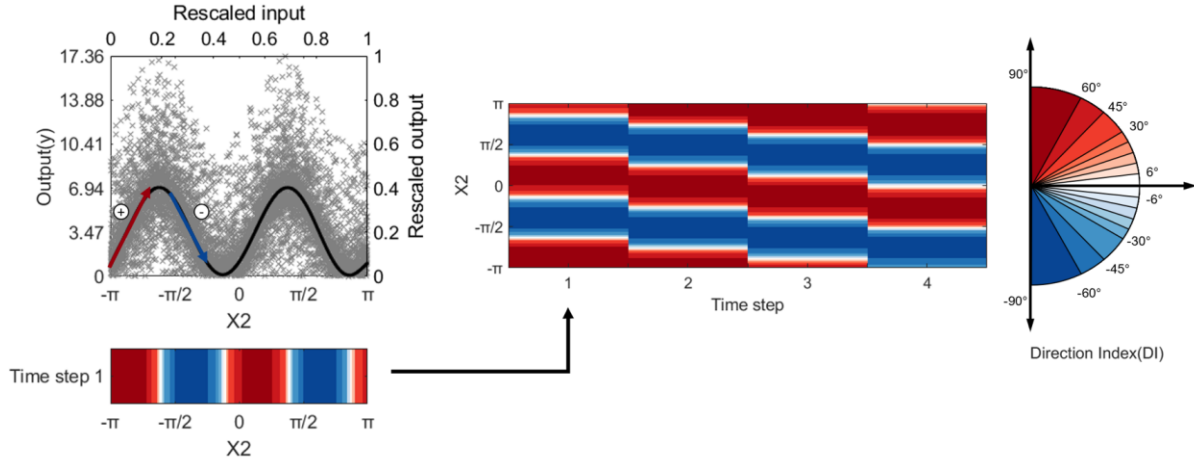


Figure 1. Demonstration example of the approximation and visualization of Direction Indices (DI plot). The top left plot shows the scatter plot of the output samples against the selected input (grey dots), together with the sum of the zeroth and first order term of the HDMR decomposition $f_i(x_i) + f_0$ (black line) for the first time step. The colormap below represents the DI of x_2 along the variability range of x_2 . The colormap on the right represents the DI of x_2 for all four time steps (horizontal axis) along the range of x_2 (vertical).

Figure 1 depicts the DI approximation result for x_2 . When DI has a positive sign, for example when x_2 increases from $-\pi$ to $-3/5\pi$, the input subrange is coloured in red, while when DI is negative, such as when x_2 changes from $-3/5\pi$ to $-1/10\pi$, the subrange is coloured in blue. The DI value varies between -90° and 90° , as shown in the legend on the very right of the figure. When the DI of the whole time series is shown, as in the central plot, the range of input variability is moved from the horizontal to the vertical axis. Here, the value of DI varies as the value of x_2 increases from the bottom to the top of the plot. In this example, we can observe that the sequence of ascending and descending trends of the output following the increases of x_2 is clearly captured in the colormap.

2.7 Approximation of first-order Sobol' Indices using the HDMR

While the approximation procedure described in Sec. 2.3-2.5 has as primary objective the calculation of the Direction Indices, an interesting and straightforward addition is the approximation of first-order Sobol' indices [Sobol', 1990, 1993, 2001]. The method of Sobol', or variance-based method, is a widely used GSA method, whereby the output sensitivity to a given input is measured by the contribution to the output variance from varying that input. RS-HDMR can also be used to compute Sensitivity Indices in an efficient way. The first-order Sensitivity Indices (SI), which measures the direct effect of input x_i on the output, is calculated as:

$$S_i = \frac{V_i}{V} \quad (13)$$

Where V is the total variance of the output due to variations in the inputs and all their possible interactions, and V_i is the partial variance due to variations in each input individually.

The total variance V is obtained by:

$$V = \int_{K^n} f^2(X) dX - f_0^2 \approx \frac{1}{N} \sum_{s=1}^N f^2(X^s) - \left[\frac{1}{N} \sum_{s=1}^N f(X^s) \right]^2 \quad (14)$$

The partial variances V_i is defined by:

$$V_i = \int_0^1 f_i^2(x_i) dx_i \quad (15)$$

We already know $f_i(x_i)$ can be approximated by orthonormal polynomials, therefore V_i can also be estimated after a long derivation process proposed by *Li et al.* [2002] as follows:

$$V_i \approx \sum_{r=1}^k (\alpha_r^i)^2 \quad (16)$$

From the description shown above, we can see that the calculation of first order SI only needs a little extra effort when computing DI. We will compute both SI and DI in the following case study to see their possible relationship and difference.

3 Case study

3.1 Hydrological model

A simple and popular conceptual rainfall-runoff model, Hymod [*Boyle, 2001*] is used in this study to demonstrate the use and usefulness of Direction Indices. It is composed of a rainfall excess model proposed by *Moore* [1985] and a routing module with a series of quickflow reservoirs and a single parallel slowflow reservoir. In the rainfall excess model, the soil moisture storage capacity is described by a pareto distribution function with two parameters: the maximum soil moisture capacity SM (mm), and Beta (-), which controls the degree of spatial variability of storage capacity over the catchment. The routing module is described by three parameters. Alpha (-) defines the portion of effective rainfall that goes into the quickflow reservoir series, while the rest goes into the slowflow reservoir. Rs (dt) and Rf (dt) are the routing time coefficients for the slow- and quickflow reservoirs, respectively. The DOC of the five model parameters are assessed. The ranges of SM, Beta, Alpha, Rs and Rf are [0, 400], [0, 2], [0, 1], [10, 150] and [0, 10] respectively [*Wagner et al., 2001*]. The parameters are assumed to be independent, which is the standard assumption for Hymod. A schematic of the model structure is shown in the Supporting Information.

3.2 Study data

The model is here applied to the widely studied Leaf River Basin near Collins Mississippi, with an area of 1949 km² [*Sorooshian, 1983*]. Precipitation, evapotranspiration and discharge data from 1952-1955 with daily time step (in mm/day) are used to run the model for this demonstration study.

3.3 Experimental set-up

Samples of the five model parameters are generated using Latin Hypercube Sampling, with a sample size of 10,000 and independent uniform distributions for all parameters within the ranges defined above. As model output, we analyse the discharge volume within a moving window at each time step, which is expressed as:

$$Q_t = \sum_{i=t-w}^{t+w} Q_i^{sim} \quad (17)$$

where w is half of the window size. We set w to 15 days, hence the full window size is 31 days. The first 60 days are excluded as warm-up period for the initial states to adjust. For each time step t , the zeroth and first order term of the HDMR expansion are estimated using scripts developed by *Ziehn and Tomlin* [2009]. The maximum polynomial order is set to 10. The ratio control variate method is applied for variance reduction.

To test the dependency of our methodology to our set-up choices, different settings have been tested. Firstly, a sample set with much smaller size (1,000) is used to assess the robustness and efficiency of our method. Secondly, we used the RMSE (Root Mean Squared Error) and Actual Evapotranspiration within a moving window as alternative model outputs. Lastly, we understand that different parameters may have different length of influential periods thus window sizes should be chosen separately for each parameter [Massmann et al., 2014]. However, for the consistency of our study we choose a window size of 31 days which is appropriate for most of the parameters. Still we applied different window sizes (3, 7, 15, 61 days) to assess the possible effects of this choice on the results. All these results can be found in the Supporting Information.

4 Results and discussion

Figure 2 shows the first order Sobol' indices (denoted as SI) and Direction Indices (DI) of each parameter over the simulation period. The results show strong temporal variations in the influence of each parameter on the model output (river discharge averaged over a moving window of 31 days).

Parameter SM [mm] – the maximum soil moisture capacity – has lower SIs in general compared with other parameters (lighter grey colours in top bar). But it shows higher SIs (darker grey) in periods of rain than during dry periods. It has large, negative DIs (darker blue) for low SM values (from 0 to about 30mm), i.e. within this subrange increases in SM lead to a reduction in discharge. In dry periods, this descending trend recedes for values above 30mm (larger SM values produce the same runoff), while in wet periods the descending trend continues also for larger values of SM. This is reasonable, in fact a larger value of SM means the catchment has more capacity to hold water, thus less runoff and more evapotranspiration will be generated. The discharge stabilizes after a threshold value of SM when the soil storage is not saturated any more (though there is some interaction with parameter Beta).

Parameter Beta [-] – the shape parameter of the soil moisture storage distribution – has higher SIs in dry periods than in rain periods. It has positive DIs (red areas) most of the time, i.e. discharge generally increases with increasing beta, except in days 380-420 and 720-800, when the sign of DIs is negative for small values of beta. In the soil moisture accounting module,

larger values of beta mean that a larger proportion of the modelled catchment has smaller soil storage capacity, hence less water can be held in the soil and more runoff is generated. However, the change of water stored in the soil is minor compared to the total runoff generated in the rainy period, therefore, Beta is less influential in rainy periods compared to dry periods. We see some interesting different behaviour of Beta during some rainy periods (days 380-420 and 720-800), where very low but increasing values of Beta seem to produce more runoff. This trend might have to do with higher Beta values producing more runoff during the preceding days, though this behaviour is also not very strong.

Parameter Alpha [-] – the fraction of effective rainfall becoming quickflow – has high SIs during both high and low flow periods. However, it has a very different effects on the model output, with positive DIs (i.e. increase in discharge for increased Alpha) in high flow periods, and negative DIs (decrease in discharge for increased Alpha) in low flow periods. In general, increasing Alpha values result in more water getting diverted to the quickflow reservoir. In high flow periods, this generates more runoff in a shorter time. In low flow periods, instead, it means that the runoff quickly leaves the catchment and without sufficient rainfall to recharge the storage, there will be less runoff in the following days.

Parameter Rs [days] – the slowflow routing time – displays a pattern of SIs similar to Alpha, but with slightly lower sensitivity values. In terms of direction of change, the behaviour is opposite to Alpha, with negative DIs (blue) in high flow periods and positive (red) in low flow periods. In high flow periods, a larger value of Rs increases the routing time, hence there will be less runoff within a time window. However, in low flow periods, when there is little effective rainfall, larger routing times increase the runoff within the time window as the runoff remains in the system for longer.

Lastly, parameter Rf [days] – the quickflow routing time – has higher SI values at time steps near the peak flows. It also has negative DIs in high flow periods and positive ones in low flow periods, but with stronger variation between periods. Because the size of the moving window (31 days) largely exceeds the upper bound of Rf (10 days), the result may not capture the features of the temporal behaviour of this parameter well [Massmann *et al.*, 2014]. The results with different choices of the moving window size can be found in the Supporting Information.

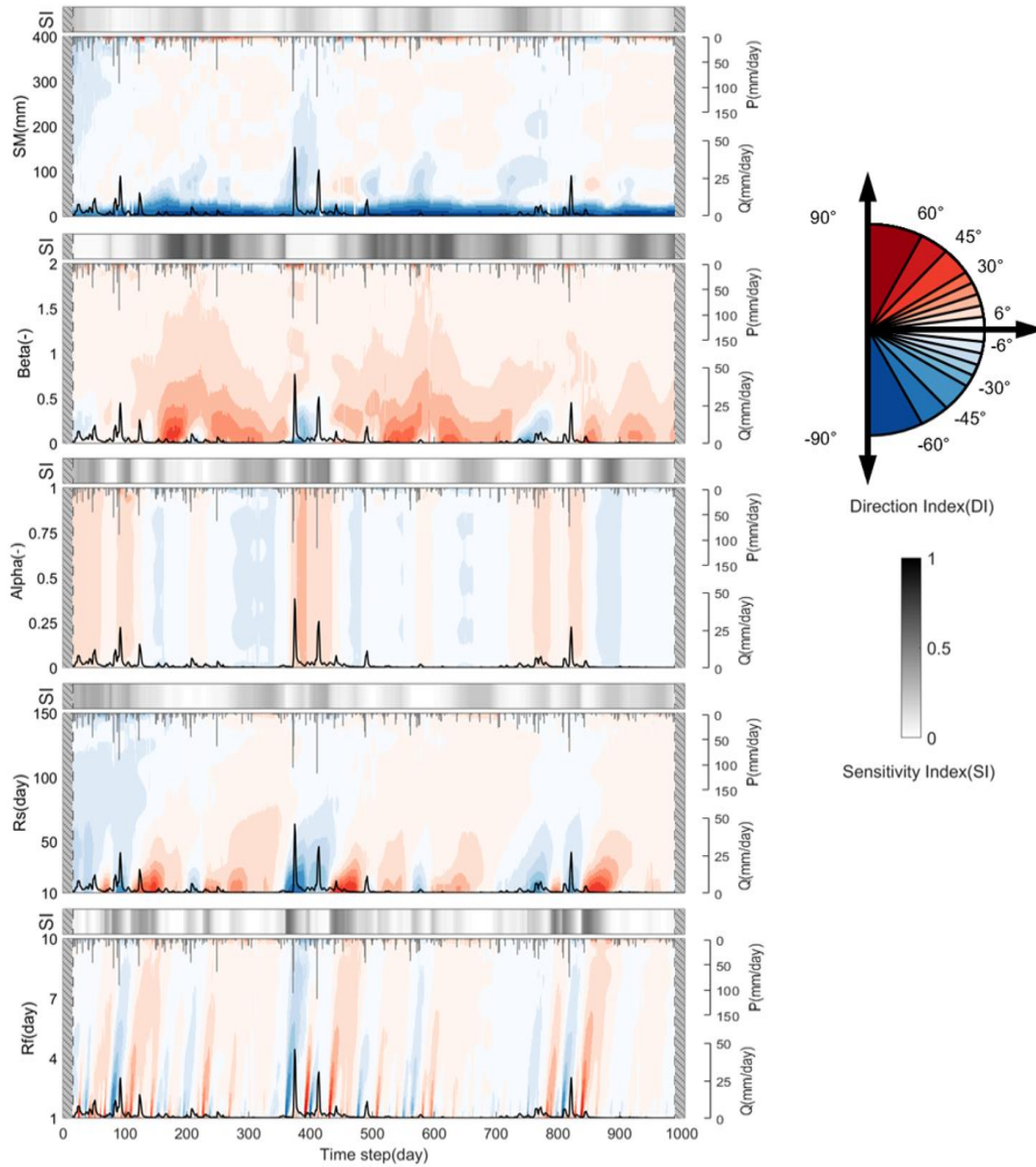


Figure 2. First order Sobol' indices (SI) and Direction Indices (DI) plots for the Hymod model applied to the Leaf catchment. Rainfall (P) and streamflow (Q) observations are shown as grey bars and black lines. The shaded parts at the beginning and end of the simulation period indicate the time steps with incomplete moving window.

These results exemplify how SI reveals which parameter is important in a certain time window, while DI reveals how the parameter controls the output in terms of DOC. Besides this, there are at least two aspects about the model behaviour that can be understood using DIs: (1) We can identify the subranges of parameter variability that influence the model output and the subranges that do not (as shown in the result of SM). In addition, the sign and absolute value of the DIs can reveal the nonlinearity and non-monotonicity of the input-output relationship (as shown in the result of SM and Beta). (2) Parameters with similar sensitivity indices (SIs) may have opposite influences on the output (as shown by the results of Alpha, Rs and Rf),

highlighting periods where the model structure creates insufficient model output variability. As shown in the previous section, the computation of both SIs and DIs can be done based on the HDMR decomposition, so the computation of DI only requires little extra calculation effort.

Our methodology illuminates some areas for model improvement. Firstly, the DI plot analyses the model structure by testing the consistency of the role of the parameters. A modeller can diagnose if the parameters control the model output in the appropriate way via the DI plot. Also, if a modeller wants to understand the behaviour of an unfamiliar model, the DI plot enables her to assess how strongly the inputs control the model output without the need to study the model structure analytically. Secondly, DI plots show how the output changes when varying each parameter, which helps in model calibration, because it provides direct guidance on the direction in which a parameter has to be changed to adjust the model output. DI plots can easily be developed for different objective functions. Lastly, in most Time-Varying SA studies, traditional SA methods (such as Sobol' or FAST) are used within a moving window to assess the model output's sensitivity to variations in the model input. These studies highlight the most sensitive or influential parameters (or parameter ranges) and try to quantify the relative "importance" of parameters. Our methodology provides complementary information to such studies. We believe "importance" (measured by SI) and "direction" (measured by DI) are complementary aspects of Sensitivity Analysis and recommend assessing both simultaneously for hydrological (or any other) models. In addition to a time-varying analysis, one could easily apply the approach also across the spatial domain of a distributed model.

5 Conclusions

We introduced a new approach to quantify and visualize the direction of change (DOC) of model outputs within a Global Sensitivity Analysis context. To this end, we presented and demonstrated a new index, called Direction Index (DI). DI is derived from the derivatives of the first order term of the high-dimensional model representation (HDMR) decomposition with respect to each input. Given the link between first order terms of the HDMR and first order terms of the variance decomposition, we can also approximate first order Sobol' sensitivity indices (SIs) while approximating our DIs. In a time-varying analysis, results can then be visualized through a colormap over the simulation period.

We demonstrated our DIs and visualisation approach by assessing the DOC for the 5 parameters of a widely used hydrological model (Hymod) in a time-varying analysis, applied to the Leaf River Catchment in the USA. We show that the joint analysis of SIs and DIs provides complementary insights. The approach is conducive to better understanding how and when the parameters (or inputs more generally) control the model output and thus offers the potential to improve the model performance by modifying the model structure or by guiding the calibration process.

In our study we provide further evidence about the additional information gained through disaggregation when mapping the input-output space of models [Wagener & Pianosi, 2019]. To conclude, we would like to point out two areas of possible future work of our study. First, the key concept of our methodology is to use a meta-model to simplify the original model and to compute the derivatives of this meta-model with respect to each input. Other meta-modelling approaches, which might be more efficient and accurate can be tested as alternatives to HDMR decomposition. Second, we use a relatively simple model to demonstrate the feasibility and utility of our methodology. Expanding our work to include more complex models would address

the need to identify suitable strategies (e.g. choose sample size and sampling method) for computationally expensive models [Gupta and Razavi, 2018] .

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The analysis reported in this study was conducted using the SAFE Toolbox (safetoolbox.info) and the GUI-HDMR scripts provided by Ziehn and Tomlin (<http://www.gui-hdmr.de/index.html>). The Matlab functions to implement the Direction Indices and the workflow script to carry out the analysis presented in this paper will be made available at <https://www.safetoolbox.info/case-studies/>.

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